

witnessCalc

A Tool for Calculating Responses of Witness Foils

By Robert Crabbs
8-12-2009

INTRODUCTION

In the interest of assaying spent nuclear fuel, we evaluate nuclear resonance fluorescence (NRF) as a possible means of identifying nuclides in a given sample. Every nuclide has a unique set of nuclear excitation energies, which can serve as a signature for the presence of that nuclide. In NRF interrogation, a continuous-spectrum photon beam is directed on a target. The photons that are very close to the excitation energies of the nuclides in the target are preferentially absorbed, and re-emitted a short time later as isotropic radiation of the same energy. Direct measurement of the output radiation at a heavily-shielded backwards angle isolates the NRF photons from the interrogating beam. The isolated NRF spectrum gives quantitative data about the composition of the target. However, NRF photons generated within the target will be heavily attenuated on the way out, resulting in low count rates at the detector.

Instead of measuring the NRF spectrum directly, we can also use a tomography-like approach to measure the effects the target has on the transmitted interrogation beam. This allows us to more accurately find the total amount of NRF absorption that occurred in the target. Since NRF radiation is emitted isotropically, the large majority of NRF photons will travel in a different direction than the original interrogating beam. A direct measurement of the transmitted beam shows how much of it was absorbed or scattered, thereby providing information on the nuclides present in the target. However, the interrogating beam itself is generally too intense for a direct measurement. Also, one is often concerned only with particular features of the output spectrum, i.e. at energies near the resonances of a specific nuclide.

A witness foil may be used to address the issues involved with direct measurement of the beam exiting the target. These foils are composed of a single type of nuclide (at least as pure as manufacturing allows), and therefore respond in a very well-defined manner to an interrogating beam. NRF in the foil is the dominant effect over an energy range comparable to the energy resolution in HPGe detectors (~ 3 keV). Therefore, one can expect significant differences in the emissions from the witness foil, depending on how the initial target affects the spectrum of the interrogation beam.

For example, consider two different targets and a test using a ^{235}U witness foil. One of the targets contains almost no ^{235}U , while the other is enriched to, say, 20%. A bremsstrahlung source creates a continuous photon spectrum with a large flux at 1.733 MeV (one of the excitation energies of ^{235}U). Unless ^{235}U is present in the target, very few of the 1.733 MeV photons in the beam interact within the target. Therefore, when this beam interacts with the low-enrichment target, it is mostly unattenuated at this key energy. When the beam then hits the witness foil, large NRF effects are observed. But in the high-enrichment target, a large fraction of the 1.733 MeV intensity is absorbed within the target. Thus, fewer of these photons remain to induce NRF within the foil. The emitted spectrum from the foil depends strongly on how much ^{235}U is present in the target.

THE PROBLEM

While it is clear that the NRF spectrum from a witness foil depends on the composition of the initial target, we need to know the relationship precisely to effectively scan nuclear material. Obtaining reliable analytical calculations is the first step towards this goal. Hand calculations for all but the simplest cases are untenable, due to the large number of nuclides involved and the complexity of cross-sections as functions of energy. MCNP seems the natural solution to get past the large amount of computation involved. However, we have recently uncovered flaws hardwired into MCNP's treatment of scattering physics. (See Brian Quiter's work on Rayleigh scattering for high-Z nuclei for a detailed description of the problem.) These flaws made MCNP unsuitable for our simulations.

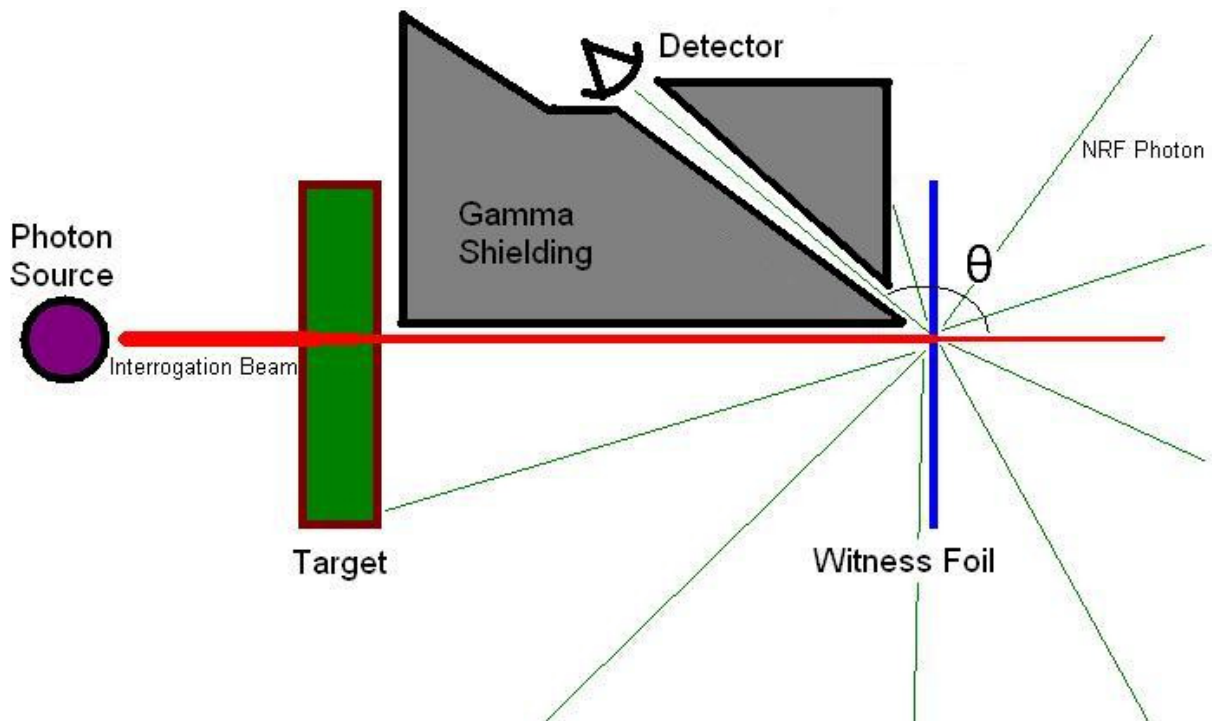


Figure 1: The Problem Geometry

THE SOLUTION

To work around these issues, we have written a set of Matlab tools designed to simulate a simple witness foil geometry. The code relies on user input for cross-section data; this allows one to include or remove various interactions at will by modifying the cross-sections. One must also specify the compositions of the target and the witness foil, among other physical parameters. A detailed description of the input can be found in the documentation section of this paper.

The toolset currently includes 6 Matlab functions:

- **witnessCalc**
This is the main control interface. It reads cross-section data from an input file, calls methods to calculate attenuation coefficients, computes output spectra, and writes the results to a text file.
- **fileReader**
Reads numerical data from a delimited text file into a matrix in Matlab. Note that the input file must be rectangular in that each line contains the same number of fields. The function skips any line containing non-numerical text.
- **parseTXTline**
A helper method for fileReader, which reads a delimited text string and returns an array of values
- **atomToMassPercent**
witnessCalc supports composition inputs in either relative atomic abundance or in mass percent. Since it is often easier to compute atomic abundances, this function converts the composition into mass percent form. This form is then directly used for calculating photon attenuation within both the target and foil.
- **attenuator**
This function takes composition and cross-section data to compute attenuation coefficients as functions of energy.
- **writeDataToTxt**
Matlab's data output is remarkably clunky and ill-suited for text files. This function allows one to more easily print data arrays directly to a specified text file.

COMPUTATIONAL METHODS

To compute the intensity of photons emitted by the witness foil, we must find the attenuation of the interrogation beam through each material. Suppose that a nuclide n_i has a cross-section function $\sigma_i(E)$ and a number density of N_i atoms per unit volume. Then the attenuation coefficient as a function of energy is

$$\mu_i(E) = \sigma_i(E) N_i$$

The total attenuation coefficient for the material is $\mu(E) = \sum \mu_i(E)$ summed over all nuclides present.

Then, given an incident photon intensity of $I_0(E)$, the attenuated intensity of the output beam is

$$I(E) = I_0(E) e^{-\mu(E) x}$$

Where x is the length of the path the beam follows through the material. For normal incidence, x is simply the thickness of the material.

Note that the number density of nuclide n_i can be calculated from its atomic mass and the density of the solid material it is part of. Specifically, if ρ is the density of the material, A_i is the atomic mass, and M_i is the mass percent of the nuclide within the material,

$$N_i = (\rho N_A M_i / 100) / A_i$$

where $N_A = 6.022 \times 10^{23}$ is Avogadro's number. The atomic abundance M_i' is related to the mass percent M_i by the formula

$$M_i = A_i M_i' / M$$

Where $M = \sum A_i M_i'$ summed over all nuclides present.

For our purposes, we assume the following geometry. The interrogating beam is incident normal to the target, which has a thickness D_1 and attenuation coefficients $\mu_1(E)$. Therefore, the spectrum of photons leaving the target (and hence which are incident on the witness foil) is defined by

$$I_{\text{to foil}}(E) = I_0(E) e^{-\mu_1(E) D_1}$$

This beam then interacts within the foil, producing NRF photons. Note that elastic scattering can also play a significant role in the detected signal. While elastic scattering cross-sections are generally very low compared to those for NRF, we will only see NRF across a narrow energy range (several eV). The energy resolution of an HPGe detector is on the order of 3 keV, so elastic scattering within 1500 keV of the resonance will contribute to the total detected peak. We may also have inelastic backscattering from higher-energy source photons, but this has not been accounted for in our programming yet.

Assume that the effects from NRF and elastic scattering can be linearly superposed. That is, let

$$I_{\text{NRF}}(E) = I_{\text{to foil}}(E) (1 - e^{-\mu_2(E) D_2})$$

given a foil thickness D_2 and attenuation coefficients $\mu_2(E)$. Similarly, define the elastic scattering intensity as

$$I_{\text{elastic}}(E) = I_{\text{to foil}}(E) (1 - e^{-\mu_3(E) D_2})$$

At this point it is essential to account for the solid angle Ω that the detector makes relative to the foil. Since NRF is emitted isotropically, we can multiply by $\Omega / 4\pi$ to get the fraction of NRF that heads toward the detector. For elastic scattering, which is decidedly not isotropic in nature, one must use the differential cross-section. One can easily factor in solid angle for elastic scattering by putting

$$\mu_3(E) = \Omega (d\sigma_i(E)/d\Omega) N_i$$

This approach assumes that the detector solid angle is small enough that the elastic scattering flux across the detector surface is constant.

The beam of photons that heads towards the detector has a total intensity of

$$I_{\text{out}}(E) = I_{\text{NRF}}(E) + I_{\text{elastic}}(E)$$

However, this output spectrum is itself attenuated as it exits the foil towards the detector. Since the NRF and elastic emissions occur at different depths within the foil, we must find an “average” attenuation distance. Let θ be the angle from the original beam axis in the foil to the detector. Assume that the distance to this detector is large enough relative to the thickness of the foil that θ does not change throughout the foil. By this, assume that the attenuation depth as seen by the NRF photons is constant over the whole solid angle subtended by the detector.

Define the spectrum that exits through the back of the foil as $I_{\text{transmitted}}(E)$. Then, use this quantity to define the average intensity within the foil to be $I_{\text{avg}}(E) = (I_{\text{to foil}}(E) + I_{\text{transmitted}}(E))/2$. The effective attenuation coefficient due to the witness foil is

$$\mu_e(E) = \mu(E) (1 + |\cos \theta|)^{-1}$$

Let the average attenuation depth then be defined

$$D(E) = -\mu_e(E)^{-1} \ln(I_{\text{avg}}(E))$$

Finally, the NRF + elastic scattering intensity that emerges from the foil at an angle of θ is:

$$I_{\text{final}}(E) = I_{\text{out}}(E) e^{-\mu_2(E) D(E)}$$

(Recall that μ_2 is the attenuation coefficient for NRF photons within the foil.) This final intensity is the signal we expect to see near the resonance.

A NOTE ON CROSS-SECTIONS

The witnessCalc toolset requires manual input of cross section data in a comma-separated value (*.csv) file. The precise format of this file will be discussed below in the documentation section. For now, we will discuss the general methodology behind the cross-sections for each step of the calculation.

As explained in the previous section on computational methods, there are three general attenuation steps to consider. First, the interrogation beam interacts within a thick target material. The portion of the beam that exits this material then comes in contact with a witness foil. Part of the beam excites NRF emissions within the foil. Elastic scattering can also occur, but generally has much smaller probability at any given energy. Finally, the NRF and elastically-scattered photons exit the foil to the detector, and are attenuated while in the foil.

For the first interaction step, we want to find the total intensity of the beam passing through the target such that the photons will afterward be incident on the witness foil. Heavy shielding between the target and the foil collimates the beam, so that scattered photons do not reach the witness foil. Since photons absorbed within the target by NRF are re-emitted isotropically, the vast majority will not reach the foil either.

Note that elastic scattering is usually a negligible effect compared with either NRF or inelastic scattering. Therefore, the only interactions we count towards attenuation in the target are inelastic scattering and NRF. These are subtracted from the initial beam intensity.

The second interaction is not so much about beam attenuation as it is about NRF production. The photons produced within the foil are of interest only if they emerge with energy close to the NRF peak in question. (Consider that an HPGe detector has roughly 3 keV energy resolution.) Inelastically-scattered photons will generally fall well outside this range, especially for large backwards angles (where we place our detector). However, elastic scattering does not change a photon's energy. So, photons which elastically scatter towards the detector will register in the same energy bins as any NRF photons.

Thus, we combine the cross-sections for NRF and elastic scattering to determine the strength of the source within the witness foil.

The final attenuation step is very similar to the first. Shielding between the foil and the detector limits the angles that photons can emerge with in order to hit the detector itself. Thus, a photon that undergoes any scattering or NRF event or will most likely not reach the detector.

Again, elastic scattering is negligible compared to the other effects, and so the cross-sections for such events can be omitted from the total. The attenuation in the final step is due entirely to NRF absorption and inelastic scattering.

Now that we have addressed what cross sections should be used where, we will explain how the cross sections themselves can be obtained. We used a combination of modeling and published libraries. Mass attenuation coefficients for photon scattering can be looked up in the XCOM database, located at <http://physics.nist.gov/PhysRefData/Xcom/Text/XCOM.html>. Be careful to use the data for *inelastic* scattering only! XCOM lists these coefficients as functions of energy, in units of cm^2/g . To use them with the witnessCalc toolset, they must be converted to barns. Let $(\mu/\rho) = M$ be the mass attenuation coefficient from XCOM (cm^2/g), while σ is the

cross section, N is the number density ($\#/cm^3$), A is the nuclear mass (au), and G is Avogadro's number (g/mol). By definition, $\mu = \sigma N$. It is also clear that $\mu = \rho (\mu/\rho) = \rho M$. Therefore,

$$\sigma = \rho M / N = (A N / G) (M / N) = A M / G$$

This gives σ in cm^2 , so a final multiplication by 10^{24} yields the cross section in barns. Note that the scattering cross-sections are very nearly constant over the small energy ranges typical of NRF peaks. However, since XCOM does not list values for all energies, linear interpolation can be used to estimate.

Elastic scattering cross-sections have been tabulated in the RTAB database for a variety of nuclides. We used the recently-computed S-matrix values released by Prof. Lynn Kissel. While the tabulations are well-populated for lower energies, there remain large gaps in the data for higher energies. In particular, RTAB does not contain information for scattering at 1.733 MeV. We wrote a set of Python scripts to linearly interpolate between entries in the database, which are included in the source code at the end of this document. Note that RTAB lists differential cross-sections.

Finally, we modeled NRF cross-sections as simple Gaussian curves. For ^{235}U , the 1733 keV resonance peak has a FWHM of 1.4 eV and integrates to 36 barn \cdot eV, yielding a maximum value of 24.158 barns. The NRF curve can be modeled to as fine of resolution as desired; we used 0.1 eV.

DOCUMENTATION

This section documents the use of witnessCalc, including input/output files and command lines. As mentioned in the introduction, this toolset includes 6 Matlab functions, all of which are required to run the chain properly. Below is a complete description of the command-line use for each function.

- `[postTarg_spec,final_spec] = witnessCalc(inputTable,atomicOrMass,targ_comp,targ_thick,targ_dense,foil_comp,foil_thick, foil_dense, detectorSolidAngle,detectorAngle,output_filename)`
All parameters except output_filename are required. If output_filename is not given, no output file is written.
 - inputTable is a string that lists the name of main cross-section data file to be used. This file must be located in the current working directory in Matlab
 - atomicOrMass is a switch with two options: 'atomic' or 'mass'. This specifies if atomic abundance or mass percent was used to define compositions. Note that this option must be the same for both the foil and the target.
 - targ_comp is a three-column array detailing the composition of the target. It has the following format:
 - Column 1: 5-digit ZAID
 - Column 2: Relative composition (in atomic % or mass %)
 - Column 3: Column index in inputTable for cross-section data for the nuclide
 - targ_thick simply gives the path length (in cm) of the beam through the target
 - targ_dense is the mass density of the target material, in g/cm³
 - foil_comp has similar form to targ_comp, but specifies the foil composition. Note that it has 5 columns, to account for the extra complexity of the interactions within the foil:
 - Column 1: 5-digit ZAID
 - Column 2: Relative composition (in atomic % or mass %)
 - Column 3: Column index in inputTable for NRF cross-section data for the nuclide
 - Column 4: Column index in inputTable for elastic scattering cross-section data
 - Column 5: Column index in inputTable for NRF + inelastic cross-section data
 - foil_thick is the thickness of the witness foil in cm
 - foil_dense is the mass density of the foil material, in g/cm³
 - detectorSolidAngle is the solid angle subtended by the detector, in steradians
 - detectorAngle is the angle between the interrogating beam direction and the line from the witness foil to the detector
 - output_filename is a string specifying the name of a tab-delimited text file to write output data to

Output values

- postTarg_spec is the relative intensity (I_{to_foil}/I_0) of the photon beam that leaves the back of the target and is thus incident on the target.
- final_spec is the relative intensity of the NRF lines that exit the witness foil. It is given in (I_{final}/I_0) / steradian.

Both output values are given as column vectors. The output written to output_filename includes a 5-column array of the form:

- Column 1: Energy (eV)

- Column 2: Source Intensity (in $\#/cm^2/s/eV$)
- Column 3: Bin width for the current row, in eV
- Column 4: postTarg_spec (normalized to source intensity)
- Column 5: final_spec (normalized to source intensity, per steradian)
- Column 6: Absolute NRF spectra leaving the foil (per steradian)

In addition, the compositions and physical parameters for the foil and target, and a copy of inputTable are included.

- `dataArray = fileReader(filename,spacingChar)`
The filename parameter is required; spacingChar is optional and defaults to ',' if not specified.
 - filename is a string giving the name of a text file to read into Matlab's memory.
 - spacingChar represents the character used to delimit the text file. '\t' (tabs) and ',' (commas) are the most common.
 - dataArray is the Matlab matrix of numerical data as retrieved from the file in question.

Note that inputTable must be a *.csv file within this toolchain. fileReader is called using the default comma delimiter.

- `[dataFields] = parseTXTline(line,spacingChar)`
The filename parameter is required; spacingChar is optional and defaults to ',' if not specified.
 - line is a delimited text string to separate into a vector of fields
 - spacingChar represents the character used to delimit the text file.
 - dataFields is a Matlab vector of string data as retrieved from the text line in question.
- `massPerc = atomToMassPercent(atomPerc)`
 - atomPerc is a composition array, as used by witnessCalc. It contains 3 columns as follows:
 - Column 1: 5-digit ZAID
 - Column 2: Relative composition (in atomic %)
 - Column 3: Column index in inputTable for cross-section data for the nuclide
 - massPerc is the same composition array as atomPerc, except that column 2 now lists the composition in mass percents
- `coefficients = attenuator(composition,density,masterArray)`
 - composition is a three column array with the standard form used for compositions in this toolset. The columns are:
 - Column 1: 5-digit ZAID
 - Column 2: Relative composition (in mass %)
 - Column 3: Column index in inputTable for cross-section data for the nuclide
 - density is the material mass density of the material through which a beam is attenuated
 - masterArray is the numeric array of cross-sections as functions of energy, as read from inputTable in witnessCalc
 - coefficients is a vector of attenuation coefficients as a function of energy
- `writeDataToFile(filename,spacingChar,varargin)`
 - filename is a string that gives the name of the file to write output data to.

- spacingChar specifies the delimiting character to write the output with
 - varargin can be any number of cells, strings, or arrays to be written to an output file.
- Note that newlines are automatically inserted between each dataset given in varargin. To insert special characters or extra delimiters, one must write them directly into the arrays.

The main cross-section data is taken from a comma-separated value (*.csv) file whose name is specified by the inputTable argument in witnessCalc. The structure of this file is as follows:

- Column 1: Energy in keV
- Column 2: Interrogation beam intensity, in $\#/\text{cm}^2/\text{s}/\text{eV}$
- Column 3: Bin width for the current row, in eV
- Columns 4+: Cross-sections (in barns) for the nuclides used in the calculation

EXAMPLE USE

To illustrate the use of witnessCalc, here is an example computation. The inputs below are written in the form one would use in Matlab.

```
targ_comp =
    [8016,55.1,7;40090,17.2,6;92238,27.7,4];

foil_comp = [92235,100,5];

[postTarg_spec,final_spec] =
    witnessCalc('masterArray.csv','atomic',targ_comp,21.8,4,foil_comp,0.5,19.1,135,
    'witnessCalcData.txt');
```

Here, the target is composed of 55.1% ^{16}O , 17.2% ^{90}Zr , and 27.7% ^{238}U by atomic abundance. Similarly, the foil is 100% pure ^{235}U . The target is 21.8 cm thick and has density $4\text{ g}/\text{cm}^3$. The foil is 5 mm thick and has a density of g/cm^3 . The detector is at a backwards angle of 135° . Finally, all output is written to a file called witnessCalcData.txt in the current working directory.

The compositions above state that the cross section data for ^{16}O can be found in column 7 of 'masterArray.csv'. Similarly, ^{90}Zr cross sections are in column 6, while those for ^{238}U and ^{235}U are in columns 4 and 5, respectively.

In addition, the masterArray.csv file might be:

```
Energy (eV),Intensity (#/eV),binWidth (eV),U-238 XS (b),U-235 XS (b),Zr-90 XS (b),O-16 XS (b)
1731500,1e9,1498,2,2,2,2
1732998,9e8,1,2,2.5,2,2
1732999,9e8,1,2,5,2,2
1733000,9e8,1,2,10,2,2
1733001,9e8,1,2,5,2,2
1733002,9e8,1,2,2.5,2,2
1734500,8e8,1498,2,2,2,2
```

In more readable form, this translates to:

Energy (eV)	Intensity (#/eV)	binWidth (eV)	U-238 XS (b)	U-235 XS (b)	Zr-90 XS (b)	O-16 XS (b)
1731500	1.00E+09	1498	2	2	2	2
1732998	9.00E+08	1	2	2.5	2	2
1732999	9.00E+08	1	2	5	2	2
1733000	9.00E+08	1	2	10	2	2
1733001	9.00E+08	1	2	5	2	2
1733002	9.00E+08	1	2	2.5	2	2
1734500	8.00E+08	1498	2	2	2	2

This table shows that ^{235}U has an NRF peak of 10 barns centered at 1.733 MeV, where the initial beam intensity gives $9.00\text{E}+08$ photons/cm²/s. Note that in the first and last bins, which are much wider than the others, many more photons are created. This allows one to weight the spectrum appropriately to deal with extremely fine energy resolution and bulk bins at the same time.

RESULTS

The first set of computations from witnessCalc focus on the form of the NRF cross-section for ^{235}U at 1733 keV. We modeled three functions for this task:

- A finite rectangle, with a 25.7-barn height and 1.4 eV width
- A Gaussian with a 24.16-barn peak and 1.4 eV FWHM
- A pyramidal shape, made from four line segments. The segment endpoints were defined by the values of the Gaussian fit at 1729 keV, 1731 keV, 1733 keV, and 1735 keV. This yielded a peak of 17.88 barns

Note that all three functions integrate to $36 \text{ eV} \cdot \text{barns}$.

These three models help illustrate the effects of approximations on the detected NRF spectra. We computed very different behavior for these functions over a range of target enrichments.

In our computations, the source had a strength of $10^{10} \text{ photons}/(\text{eV} \cdot \text{s} \cdot \text{cm}^2)$ over the entire range of interest--specifically $1733 \pm 1.5 \text{ keV}$ (approximately the resolution of an HPGE detector). The target contained 27.7% uranium, 55.1% oxygen, and 17.2% Zr by atomic abundance. This is a much simplified composition representing LWR spent fuel in a zirconium storage matrix. The target itself was a uniform 21.8 cm thick with a density of 4.0 g/cm^3 . We varied the composition of the target by varying the enrichment of ^{235}U , while assuming that the oxygen and zirconium retained their natural isotopic abundances. Note that ^{235}U and ^{238}U are the only isotopes of uranium we considered. We computed data for enrichments of 0%, 0.5%, 1%, 5%, 10%, 25%, 50%, and 100% ^{235}U .

The witness foil was composed of pure ^{235}U , with a density of 19.1 g/cm^3 . We compared two thicknesses: 1 mm and 5 mm. Also note that we assumed a detector positioned at a backwards angle of 135° , subtending a solid angle of 0.0053 steradians.

A computation was carried out for every combination of target enrichment, NRF cross-section model, and foil thickness, resulting in 48 runs total. We plotted two sets of data from these runs:

- Total detected countrate as a function of target enrichment
- Ratio of NRF photons vs. elastically scattered photons incident on the detector, as a function of target enrichment

Both plots are normalized to the results for 0% target ^{235}U enrichment.

The detected countrate is defined as the total number of photons that are incident upon the detector; it is the sum of the "Absolute Detected Intensity (counts/s)" column given in a witnessCalc output file. As discussed in the "Notes on Cross Sections", NRF is the dominant effect close to the NRF peak, though rarer elastically-scattered photons can significantly affect the detected rate over a 3 keV energy range. (For comparison, NRF only acts over a range of a few eV.)

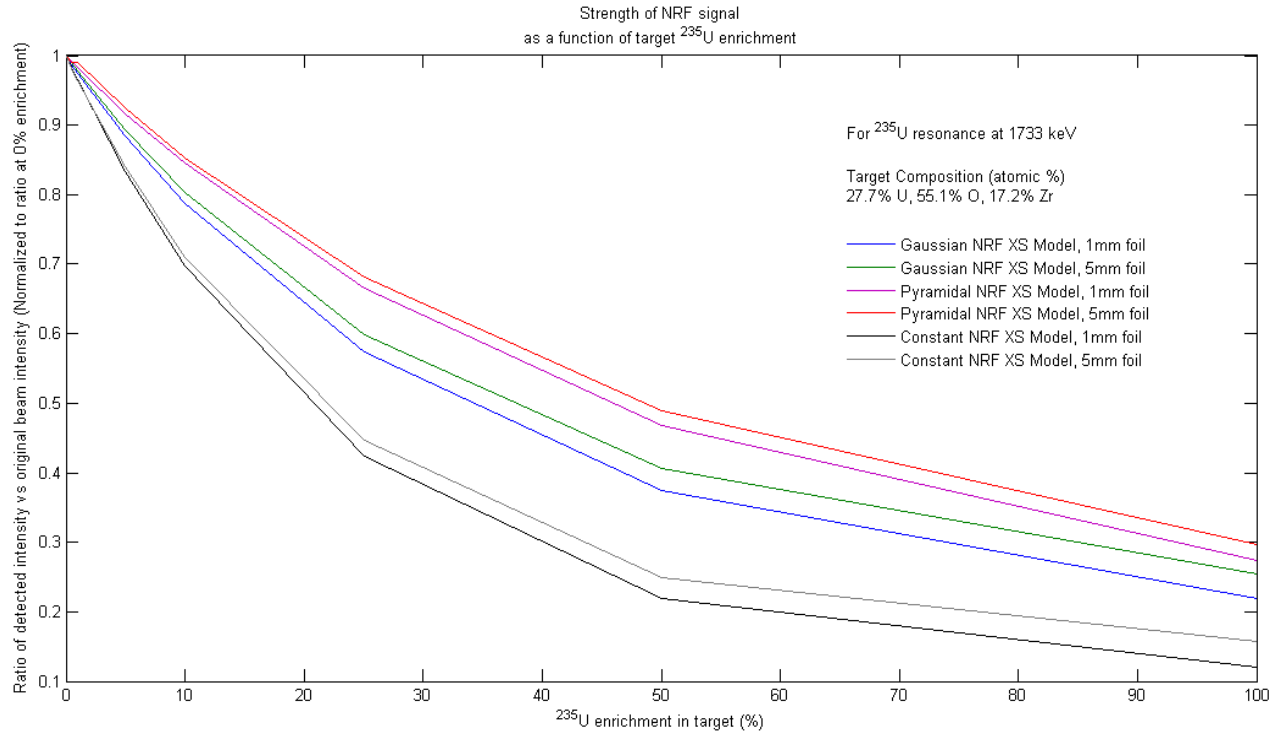


Figure 2: Detected count-rate as a function of target enrichment

Figure 2 shows a marked correlation between target composition and the number of resonant-energy photons incident upon the detector. In general, we note a roughly exponential decrease in the detected count rate as enrichment increases from 0% to 100%.

The six curves correspond to the different cross-section models for both 1 mm and 5 mm witness foil thicknesses. The thicker foil yields higher countrates within the detector, as expected. The very high concentration of ^{235}U in the foil makes NRF very much the dominant effect here. The countrates are not increased by a factor of 5, however, because of resonant attenuation within the foil itself.

Note that the square NRF cross-section model resulted in the lowest number of counts within the detector.

The NRF signal was on the order of 10^{-12} as strong as the original interrogation beam. For a source strength of 10^{10} photons/(eV \cdot s \cdot cm 2), we obtain a total detected yield of $\sim 30,000$ counts/s.

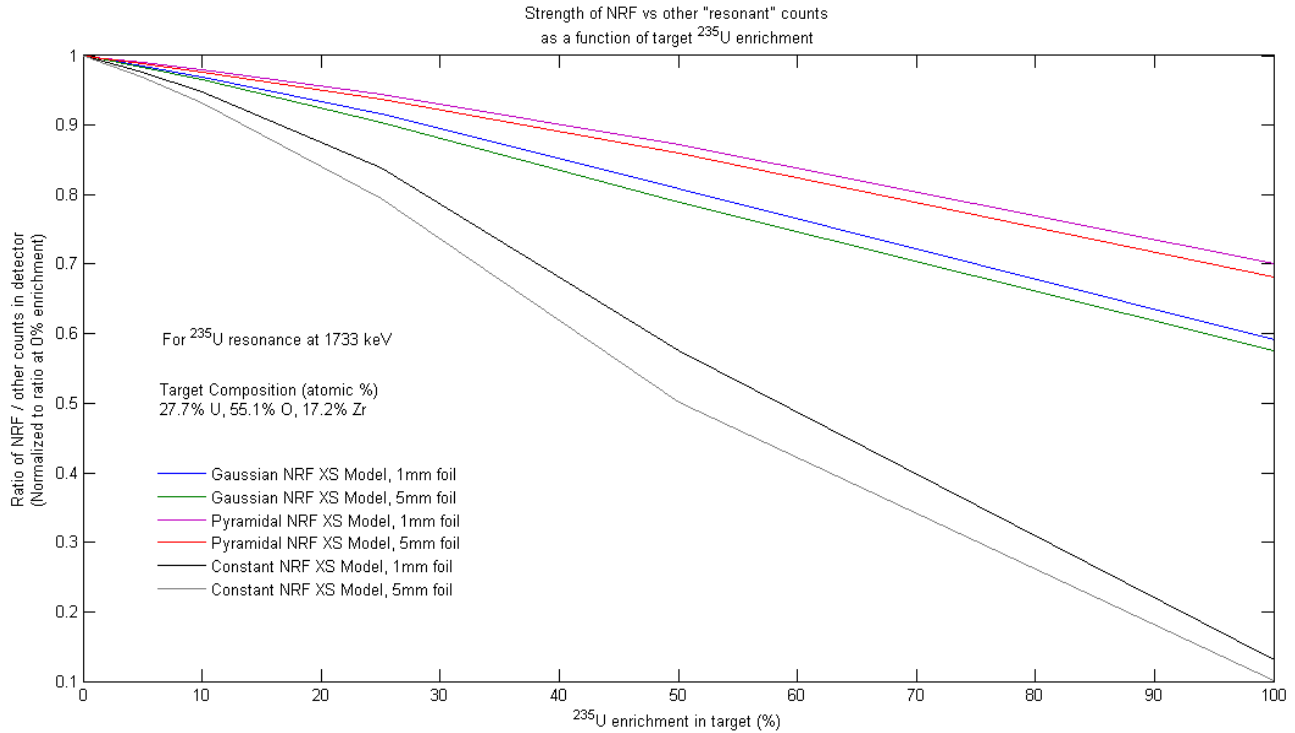


Figure 3: Ratio of NRF photons vs. elastically scattered photons incident on the detector

Figure 3 illustrates how elastic scattering becomes more significant for the output signal as target enrichment increases. This makes sense, noting that resonant photons tend to die off quickly due to a high absorption cross section. Therefore, far fewer photons within 1-2 eV of the NRF peak pass through the target to excite fluorescence within the foil. Since elastic scattering has a very small cross-section in comparison, photons within 1-2 keV of the peak generally reach the foil. These can then elastically scatter to the detector, contributing to the signal.

Note that the data for the square cross-section model drops off rather sharply compared to that from the other two models.

Further Work

Now that we have demonstrated a successful computational method in the witnessCalc toolchain, we can use it to simulate more complicated compositions. This will, of course, allow us to better predict results of upcoming experiments.

Our initial work used a single target thickness so as to study the effects of cross-section approximations. The next step may be to vary the thickness of a target of standard composition. There are far too many conceivable geometries and compositions to simply compute signature spectra for each. It would be far better to obtain an analytical expression predicting such spectra as functions of composition and target thickness.

We are also interested to find the foil thickness which maximizes our NRF countrate, which determines the precision with which we can identify the target.

REFERENCES

NIST XCOM – Photon Cross Section Database. National Institute of Standards and Technology, Physics

Laboratory. <http://physics.nist.gov/PhysRefData/Xcom/Text/XCOM.html>

Lynn Kissel, RTAB: the Rayleigh scattering database, Radiation Physics and Chemistry, Volume 59, Issue 2, 1 August 2000, Pages 185-200

Matlab Online Documentation. The Mathworks.

<http://www.mathworks.com/access/helpdesk/help/helpdesk.html>

Python Documentation. Python Software Foundation. <http://www.python.org/doc/>

SOURCE CODE

The source code for witnessCalc, fileReader, parseTXTline, atomToMassPercent, attenuator, and writeDataToTxt is given below, along with the scripts dealing with the RTAB database.

writeDataToFile.m

Allows one to more easily print data arrays directly to a specified text file

```
function writeDataToFile(filename,spacingChar,varargin)
% Function writes a tab-delimited file from data specified in varargin
% -- "filename" is the name of the file to be written
% -- "spacingChar" determines how the data fields in each object passed
%    through varargin should be spaced. For example, if spacingChar = '\t',
%    then the output file will be tab delimited.
% -- varargin contains any number of headers and/or data matrices to write
%    to a file. This function decides what each parameter is and prints it
%    appropriately.
fileID = fopen(filename,'wt');

% First, we determine how many objects there are to print
for i = [1:length(varargin)]
    data = varargin{i};
    % Matlab is very clunky for dealing with file output and strings
    % We need to convert each entry in data into a string to write
    % separately.
    [rows,columns] = size(varargin{i});
    for R = [1:rows]
        temp = cell(1,columns);
        for C = [1:columns]
            temp = data(R,C); % temp is the ith row of the dataArray matrix
            if isa(temp,'numeric') == 1
                temp = num2str(temp);
            elseif isa(temp,'cell') == 1
                temp = temp{1};
            else
                error(['Undefined data type. Cannot write as text']);
            end
            % Special characters will be interpreted literally. Let's
            % interpret them if they come up:
            if strcmp(temp,'\n')
                fprintf(fileID,'\n');
            elseif strcmp(temp,'\t')
                fprintf(fileID,'\t')
            % Print the data and a tab-delimiter, unless it's the last column
            elseif C == columns % Print a newline character instead of a tab here
                fprintf(fileID,'%s\n',temp);
            else
                fprintf(fileID,'%s\t',temp);
            end
        end
    end
end
end
fclose(fileID);
```

fileReader.m

Reads numerical data from a delimited text file into memory in Matlab

```
% Reads numerical data from a *.csv file into memory
% This function automatically removes any lines that contain non-number
% strings. Make sure the *.csv is rectangular and only contains one dataset!
```

```
function dataArray = fileReader(filename,spacingChar)
fileID = fopen(filename);
if fileID < 0
    error(['Could not open ',filename,' for input']);
end

% If spacingChar is not specified, this reads *.csv files by default
if nargin < 2
    spacingChar = ',';
end
% First we need to figure out the dimensions of our master array.
% "rows" represents the number of rows, while "cols" is the number of
% columns
status = 1;
rows = 0;
cols = 0;
while status > 0
    line = fgetl(fileID);
    % We only want to see how many fields are in the line
    junk = parseTXTline(line,spacingChar);
    tempCols = length(junk);
    % If this line has a different number of fields than the line before it,
    % we have a problem!
    if (tempCols ~= cols && cols ~= 0 && tempCols ~= 0)
        error(['*.csv data is not rectangular']);
    end
    if line == -1
        status = 0;
        break
    end
    rows = rows + 1;
    cols = tempCols;
end
```

```
% Need to reinstantiate the *.csv file for access
fileID = fopen(filename);
```

```
% strArray is a cell whose entries represent the columns in the *.csv file
% It is output as a cell of strings
strArray = cell(rows,cols);
```

```
% This loop populates strArray and then checks to see which rows have
% non-number strings in them
badRows = []; % Contains the row indices for the non-number strings
for i = [1:rows]
    line = fgetl(fileID);
    NaNFlag = 0;
    [data,junk] = strtok(line,',' );
    % Now we parse the data by comma-delimiting
    fields = parseTXTline(data,spacingChar);
    for j = [1:cols]
        % Is the data point not a valid number?
        if size(str2num(fields{j})) == [0 0]
            NaNFlag = 1; % True if one or more entries is NaN
        end
    end
end
```

```

        strArray{i,j} = fields{j};
    end
    % If we found a non-number, we'll skip the row for the final array
    if NaNFlag == 1
        badRows = [badRows i];
    end
end
end

% We have now read the *.csv file into memory. Now we want to take out
% header rows or any other rows containing text
[junk,rowsToDel] = size(badRows);
dataArray = zeros(rows-rowsToDel,cols);
index = 1;
for i = [1:rows]
    % Checking if badRows contains the current row index
    % Only writes good rows to dataArray
    if size(find(badRows == i)) ~= [1 1]
        for j = [1:cols]
            dataArray(index,j) = str2num(strArray{i,j});
        end
        index = index + 1;
    end
end
end

fclose all;

```

parseTXTline.m

A helper method that separates delimited text into an array of data

```
function [dataFields] = parseTXTline(line,spacingChar)
% Uses a while loop to extract data fields from a comma-delimited string

% If spacingChar is not specified, this reads *.csv files by default
if nargin < 2
    spacingChar = ',';
end

% Want to figure out how many data entries there are, first
% This loop finds the first field from the string, then loops using the line
% minus that field
counter = 0;
tempLine = line;
while length(tempLine) > 1
    [field,remainder] = strtok(tempLine,spacingChar);
    tempLine = remainder;
    counter = counter + 1;
end

dataFields = cell(1,counter);
% Must reinitialize the line to read into dataArray
tempLine = line;
for i = 1:counter
    [field,remainder] = strtok(tempLine,spacingChar);
    tempLine = remainder;
    dataFields{i} = field;
end
```

atomToMassPercent.m
Converts compositions from atomic abundances to mass percents

```
function massPerc = atomToMassPercent(atomPerc)
% Converting composition arrays from atomic percent to mass percent

% This function converts the material composition given by the
% atomPerc matrix, specified in atomic percentages, into the
% masses matrix. The output lists the composition in terms of mass
% percents.

% The input matrix should have two columns: the first gives ZAIDs for the
% component nuclides, while the second gives the atomic percentage within
% the material in question.

[nuclides,columns] = size(atomPerc);

% massPerc has an identical structure to atomPerc. Only column 2 is
% different
massPerc = atomPerc;
masses = zeros(nuclides,1);

totalAtomPercent = 0; % A quick check to make sure the composition was normalized correctly
for i = [1:nuclides]
    % What is the number density of the nuclide?
    ZAID = atomPerc(i,1);

    Z = double(uint16(ZAID/1000));
    A = ZAID - Z*1000;
    atomPercent = atomPerc(i,2);

    totalAtomPercent = totalAtomPercent + atomPercent;

    % Now to find the weighted mass proportions
    masses(i) = atomPercent*A;
end

% The total mass is the sum of all entries in masses; this lets us
% compute mass percents
totalMass = sum(masses);
massPerc(:,2) = 100*masses/totalMass;

if totalAtomPercent ~= 100
    sprintf('Warning: An atomic composition is not normalized to 100 percent!\nIt sums to %f
percent.',totalAtomPercent)
end
```

attenuator.m

Computes attenuation coefficients from given compositions and cross-sections

```
function coefficients = attenuator(composition,density,masterArray)
% Used in tandem with witnessCalc to compute attenuation coefficients

% The input requires the composition, density, and thickness of the
% material through which a beam is attenuated. In addition, a masterArray
% contains all the cross-section data for the nuclides specified in the
% composition matrix.

%
% -- composition is a three-column matrix specifying the composition of the
% target. The first column should list ZAIDs while the second lists the
% relative abundance of nuclides (in mass %). The third column points to
% the column in inputTable that contains cross-section data for the
% nuclide.
% -- density is the density of the target in g/cc

% masterArray has the following structure:
% Column 1: Bin energy in keV
% Column 2: Intensity of the source as a function of energy within each bin
%           (in units of #/s/cm^2/eV for normalization)
% Column 3: Widths of the energy bins in column 2 (in eV)
% Columns 4+: Cross-sections of nuclides in the target or foil as a
%             function of energy (in barns)

[N_bins,columns] = size(masterArray); % Looks up how many energy bins there are

% Need to find the size of targ_comp to know how many nuclides are present
[nuclides,columns] = size(composition);

% The number of interactions in the target as a function of E, per unit time
coefficients = zeros(N_bins,1);

totalMassPercent = 0; % A quick check to make sure the composition was input correctly
for i = [1:nuclides]
    % What is the number density of the nuclide?
    ZAID = composition(i,1);
    Z = double(uint16(ZAID/1000));
    A = ZAID - Z*1000;

    massPercent = composition(i,2);

    N_density = (6.022*10^23)*(density*massPercent/100)/A;

    % Where is the cross-section data in masterArray?
    xs_col = composition(i,3);
    nuclide_xs = 10^-24*masterArray(:,xs_col);

    % Each individual component of the target contributes to the effective
    % cross section, and hence the attenuation coefficient:
    coefficients = coefficients + N_density*nuclide_xs;
end
```

witnessCalc.m

```
function [postTarg_spec,detected_spec] =  
    witnessCalc(inputTable,atomicOrMass,targ_comp,targ_thick,targ_dense,foil_comp,foil_thick,foil_dense,  
    detectorSolidAngle,detectorAngle,output_filename)  
% Function for calculating the response spectrum from a witness foil  
  
% A gamma source (whose distribution is defined in inputTable) is normally incident  
% upon a target that may or may not interact with the beam via NRF. The  
% photons which do not interact in the target then hit a witness foil,  
% which gives off a spectrum which depends on the composition of the target  
  
% -- inputTable is the filename of a *.csv file containing a gamma source  
% distribution. Structure is detailed below  
% -- atomicOrMass specifies if input compositions list data in atom vs mass  
% percents. It can have two values: 'atomic' or 'mass'  
% -- targ_comp is a three-column matrix specifying the composition of the  
% target. The first column should list ZAIDs while the second lists the  
% relative abundance of nuclides (in atom or mass %). The third column  
% points to the column in inputTable that contains cross-section data  
% for the nuclide.  
% -- targ_thick is the thickness of the target material in cm.  
% -- targ_dense is the density of the target in g/cc  
% -- foil_comp is the same as targ_comp, but gives information about the  
% foil instead of the target  
% -- foil_thick is the thickness of the witness foil material in cm.  
% -- foil_dense is the density of the foil in g/cc  
% -- detectorSolidAngle is the solid angle subtended by the detector, in  
% steradians  
% -- detectorAngle is the backward angle at which the detector sits  
% relative to the foil  
% -- If output_filename is given, witnessCalc will write the post-target  
% and final NRF spectra to that file in tab-delimited format. Otherwise,  
% no output file will be written.  
  
% inputTable has the following structure:  
% Column 1: Bin energy in keV  
% Column 2: Intensity of the source as a function of energy within each bin  
% (in units of #/s/cm^2/eV for normalization)  
% Column 3: Widths of the energy bins in column 2 (in eV)  
% Columns 4+: Cross-sections of nuclides in the target or foil as a  
% function of energy (in barns)  
  
% Need a copy of csvReader for this to work  
masterArray = fileReader(inputTable);  
  
srcEnergies = masterArray(:,1); % Source spectrum particle energies  
binWidths = masterArray(:,3);  
srcIntensity = masterArray(:,2).*binWidths; % Source spectrum strength: counts/s/cm^2  
  
if strcmpi(atomicOrMass,'atomic') == 0 && strcmpi(atomicOrMass,'mass') == 0  
    error(['Specify whether compositions are given in atomic percents or mass percents!'])  
else if strcmpi(atomicOrMass,'atomic') == 1  
    targ_comp = atomToMassPercent(targ_comp);  
    foil_comp = atomToMassPercent(foil_comp);  
end  
end  
  
% Transport of the source beam will happen in three steps:  
  
% First, the source spectrum is attenuated due to the target
```

```

targ_atten_coeffs = attenuator(targ_comp,targ_dense,masterArray);
postTarg_spec = srcIntensity.*exp(-targ_atten_coeffs*targ_thick);

% Next, the beam that goes through the target unscattered will be incident
% on the witness foil. The NRF spectrum produced within the foil is equal
% to the total number of NRF and elastic scattering interactions.
% We need to use different cross-sections for NRF production versus the
% attenuation of the NRF spectra on its way out the foil.

% foil_comp should have five columns. Columns 3-5 point to columns in
% masterArray that contain cross-section data. Column 3 is solely for NRF,
% column 4 is for elastic scattering, and column 5 is for all interactions
% that attenuate the NRF photons in the foil (i.e. NRF + inelastic).

NRF_comp = foil_comp(:,1:3);

% Defining the composition array for elastic scattering
% This array is the same as NRF_comp except for the last column
elastic_comp = NRF_comp;
elastic_comp(:,3) = foil_comp(:,4);

NRF_prod_coeffs = attenuator(NRF_comp,foil_dense,masterArray);
initial_NRF_spec = postTarg_spec - postTarg_spec.*exp(-NRF_prod_coeffs*foil_thick);
% Must factor in the solid angle of the detector. Assume NRF radiates
% isotropically.
initial_NRF_spec = initial_NRF_spec * detectorSolidAngle / (4*pi);

% To factor in solid angle for elastic scattering, we multiply the elastic
% scattering cross-section (given in barns per steradian) by the solid
% angle of the detector. attenuation coefficients depend linearly on
% cross-section
elastic_coeffs = attenuator(elastic_comp,foil_dense,masterArray)*detectorSolidAngle;
elastic_spec = postTarg_spec - postTarg_spec.*exp(-elastic_coeffs*foil_thick);

% The final attenuation step is through the foil to the detector. The foil
% attenuates the NRF_spec on its way out. We assume the thinness of the
% foil is sufficiently small compared to the distance to the detector that
% it does not affect the scattering angle.
% The interaction depth is also not constant within the foil; we'll need to
% calculate an average attenuation depth to determine what distance to
% attenuate over. Define the average *interaction* distance to be the depth
% for which the attenuated spectrum is halfway between the input and the
% output through the back of the foil. The average *attenuation* depth
% also accounts for the backwards-scattered attenuation of the NRF spectrum
% through the foil.
% Note the dependence of attenuation depth on photon energy.

% The total spectrum that heads in the direction of the detector:
NRF_elastic_spec = initial_NRF_spec + elastic_spec;

% The spectrum that exits the back of the foil without interaction
% We multiply by the solid angle again to account for ALL the NRF
% interactions, not just the ones that head towards the detector
postFoil_spec = postTarg_spec - (initial_NRF_spec*4*pi/detectorSolidAngle + elastic_spec);

avgIntensity = (postFoil_spec + postTarg_spec)/(2*postTarg_spec);
detected_spec = zeros(length(NRF_elastic_spec),1); % The spectrum that will be incident on the detector

% Defining the composition array for use in the final attenuation step
% This array is the same as NRF_comp except for the last column, which
% specifies cross-sections for all interactions that will attenuate the
% NRF on its way out

```

```

foil_atten_comp = NRF_comp;
foil_atten_comp(:,3) = foil_comp(:,5);

foil_atten_coeffs = attenuator(foil_atten_comp,foil_dense,masterArray);

for i=[1:length(avgIntensity)]
    if foil_atten_coeffs(i) ~= 0
        attenuation = foil_atten_coeffs(i)*(1+1/abs(cos(detectorAngle)));
        avg_depth = -log(avgIntensity(i))/attenuation;
        % avg_depth is the depth within the foil at which the intensity is
        % halfway between what was incident on the foil and what came out
    else avg_depth = log(2)*foil_thick;
    end
    detected_spec(i) = NRF_elastic_spec(i)*exp(-foil_atten_coeffs(i)*avg_depth);
end

% Lastly, divide by the source intensity to get the final spectrum due
% to NRF, independent of source. Dividing by 4*pi yields the NRF spectrum
% per steradian, assuming the detector solid angle is small enough that the
% attenuation depth within the foil is relatively constant.
% This also assumes isotropic emission.
postTarg_spec = postTarg_spec./srcIntensity;
detected_spec = detected_spec./srcIntensity;

% File output of spectra and settings if a filename is specified
if nargin > 10
    spec_header = {'Energy (eV)','Source Intensity (#/eV)','Bin Width (eV)','Normalized Post-Target Intensity',
        'Normalized Detected Intensity','Absolute Detected Intensity (counts/s)'};
    output = [masterArray(:,1:3) postTarg_spec detected_spec detected_spec.*srcIntensity];
    detector_header = {'\n','Detector Solid Angle (steradians):',num2str(detectorSolidAngle),'\n',
        'Detector Angle (degrees):',num2str(detectorAngle)};
    targ_header = {'\n','Target Composition','\n','Thickness (cm):',num2str(targ_thick),'\n',
        'Density (g/cm^3):',num2str(targ_dense)};
    targ_header2 = {'\n','ZAID','Mass Percent','XS Column'};
    foil_header = {'\n','Foil Composition','\n','Thickness (cm):',num2str(foil_thick),'\n','Density
(g/cm^3):',num2str(foil_dense)};
    foil_header2 = {'\n','ZAID','Mass Percent','NRF XS Column','Elastic Scattering XS Column','Attenuation XS'};
    masterArray_header = {'\n','Master XS Array Used'};

    writeDataToFile(output_filename,'\t',spec_header,output,detector_header,targ_header,targ_header2,targ_comp,
        foil_header,foil_header2,foil_comp,masterArray_header,masterArray);
end

```

format_RTAB.py
Creates a compact version of an RTAB table

```
# This script removes all superfluous comments from an RTAB database
input_table = open("092_cs0sl_sm+nt.txt","r")
output_table = open("compact_92_sm+nt.txt","w")

def isPosInt(string):
    status = 1
    if isSciNotation(string) == 1:
        # Check scientific notation to be an integer
        number = float(string)
        if number - int(number) != 0:
            status = 0
    # isdigit() method tests if a string is only numeric. Only integers return true
    elif isSciNotation(string) == 0 and string.isdigit() == 0:
        status = 0
    elif int(float(string)) < 1:
        status = 0
    return status

# Python knows how to use scientific notation, but we have to convert the string into a float to use it
# This method checks to see if a string can be interpreted by Python as scientific notation
def isSciNotation(string):
    status = 1
    string = string.lower()
    if string.find("e"):
        try: float(string)
        except ValueError:
            status = 0
    else:
        status = 0
    return status

# Now to start scripting
for line in input_table:
    if line.startswith("**BLOCK:") == 1:
        output_table.write(line)
    elif line.startswith(" THETA") == 1:
        output_table.write(line)
    elif line == "\n":
        output_table.write(line)
    else:
        data = line.split()
        if data != [] and isPosInt(data[0]) == 1:
            output_table.write(line)
```

interpolate_RTAB.py

Linearly interpolates between two data sets in RTAB to estimates values at arbitrary energies

This script takes data from a compact rtab table and estimates cross-sections for an arbitrary photon energy

```
#####  
### FUNCTION DEFINITIONS ###  
#####
```

```
def findNearestE(photon_energy,database):  
    input_table = open(database,"r")  
    # Initializing high/low energy values  
    # high_diff and low_diff show how close in keV the energy is to the given photon energy  
    high_E = -1; high_diff = -1  
    low_E = -1; low_diff = -1  
    for line in input_table:  
        # If the line begins with *BLOCK: then we have found the start of a data section  
        if line.startswith("*BLOCK:"):   
            temp = line.split(":")  
            temp = temp[1].split("keV")  
            # Get rid of the non-numerical tail  
            energy = float(temp[0])  
            diff = abs(energy - photon_energy)  
            # If either value is not yet defined, we'll define them.  
            if high_diff < 0:  
                high_diff = diff  
                high_E = energy  
            elif low_diff < 0:  
                low_diff = diff  
                low_E = energy  
            # If we find closer energies, we must redefine high_E and low_E  
            elif diff < high_diff or diff < low_diff:  
                low_diff = high_diff; high_diff = diff  
                low_E = high_E; high_E = energy  
    if low_E > high_E:  
        line = low_E  
        low_E = high_E  
        high_E = line  
    input_table.close()  
    return low_E,high_E
```

```
def findBoundingE(photon_energy,database):  
    input_table = open(database,"r")  
    # Initializing high/low energy values  
    high_E = -1; low_E = -1  
    for line in input_table:  
        # If the line begins with *BLOCK: then we have found the start of a data section  
        if line.startswith("*BLOCK:"):   
            temp = line.split(":")  
            temp = temp[1].split("keV")  
            # Get rid of the non-numerical tail  
            energy = float(temp[0])  
            if energy < photon_energy and energy > low_E:  
                low_E = energy  
            if energy > photon_energy and high_E < 0:  
                high_E = energy  
    input_table.close()  
    return low_E,high_E
```

```

def getDataForInterpolation(low_E,high_E,database):
    low_E_data = []; high_E_data = []
    input_table = open(database,"r")
    lowDataFlag = 0
    highDataFlag = 0
    for line in input_table:
        # Stop reading upon reaching the blank line separator between sections
        if line == "\n":
            lowDataFlag = 0
        elif lowDataFlag == 2: lowDataFlag = 1
        # Read cross-section data for low_E
        elif lowDataFlag == 1:
            low_E_data.append(line)
        # Start reading two lines after the *BLOCK: header line
        elif line.startswith("**BLOCK:" + str(low_E)) == 1:
            lowDataFlag = 2

        # Stop reading upon reaching the blank line separator between sections
        if line == "\n":
            highDataFlag = 0
        elif highDataFlag == 2: highDataFlag = 1
        # Read cross-section data for low_E
        elif highDataFlag == 1:
            high_E_data.append(line)
        # Start reading two lines after the *BLOCK: header line
        elif line.startswith("**BLOCK:" + str(high_E)) == 1:
            highDataFlag = 2

    input_table.close()
    return low_E_data,high_E_data

def interpolate(energy,low_E,low_E_data,high_E,high_E_data):
    interpolated = []
    # We're assuming that low_E_data and high_E_data are the same length
    # They should be, because RTAB gives data for each energy in a well-defined
    # angular distribution
    for index in range(0,len(low_E_data)):
        # Read in the data for each line
        # We will split it into numerical values next
        low_line = low_E_data[index]
        high_line = high_E_data[index]
        low_line = low_line.split()
        high_line = high_line.split()
        interpolated_line = []
        # First, add the angle value for this particular data
        interpolated_line.append(float(low_line[0]))
        # Now we'll find the rest of the data
        for j in range(1,len(low_line)):
            low_data_point = low_line[j].replace("\n","")
            high_data_point = high_line[j].replace("\n","")
            low_data_point = float(low_data_point)
            high_data_point = float(high_data_point)
            # Now for the linear interpolation!
            slope = (high_data_point - low_data_point)/(high_E - low_E)
            y_intercept = (low_data_point*high_E - high_data_point*low_E)/(high_E - low_E)
            interpolated_point = slope*energy + y_intercept
            interpolated_line.append(interpolated_point)
        interpolated.append(interpolated_line)
    return interpolated

# Takes an arbitrary numerical value and returns it in scientific notation with a specified number of sigFigs
def formatValue(number,sigFigs):
    number = float(number)

```

```

negativeFlag = 0
if number < 0:
    number = abs(number)
    negativeFlag = 1
# This gets our input into a standard format
# Now we avoid errors with decimals like .234 vs. 0.234
# float() also puts exponents in the right form for number < 0.0001
string = str(number).upper()
if string.find("E") == -1: # Not yet in scientific notation
    index = 0
    exp = 0
    if string.find(".") >= 1 and string.startswith("0") == 0: index = string.find(".")
    elif string.find(".") <= 1: # A decimal < 1
        # We must find the first nonzero digit
        # Since we already converted to a float in the beginning, we are limited
        # to decimals > 0.0000999999...
        if len(string) > 3 and string[2] != "0": index = -1
        elif len(string) > 4 and string[3] != "0": index = -2
        elif len(string) > 5 and string[4] != "0": index = -3
        elif len(string) > 6 and string[5] != "0": index = -4
    else: index = len(string) # For numbers without a decimal point (ints)

    if index > 0: exp = index - 1
    else: exp = index
    coeff = number/10**exp

    # If exp is a single digit, we will add a "0" in front, i.e. 1.0e-2 -> 1.0e-02
    if abs(exp) < 10:
        # Must take into account a negative sign
        if exp < 0:
            exp = "-0" + str(abs(exp))
        else: exp = "0" + str(exp)
    if int(exp) >= 0 and str(exp).find("+") == -1:
        exp = "+" + str(exp)

    # We also want to round the coefficient to an appropriate number of sig figs
    coeff = str(coeff)
    if coeff.find(".") == -1: coeff = coeff + "."
    if len(coeff) > sigFigs + 1: # +1 to account for decimal point in the string
        coeff = coeff[0:sigFigs+1]
    else:
        while len(coeff) <= sigFigs:
            coeff = coeff + "0"
    string = coeff + "E" + exp
else: # we need to now make sure of the number of sig figs
    temp = string.split("E")
    coeff = temp[0]
    if coeff.find(".") == -1: coeff = coeff + "."
    if len(coeff) > sigFigs + 1: # +1 to account for decimal point in the string
        coeff = coeff[0:sigFigs+1]
    else:
        while len(coeff) <= sigFigs:
            coeff = coeff + "0"
    string = coeff + "E" + temp[1]

if string.find("E-02") > -1 and number > 0.1:
    print(number)
    print(string)
    print("_____")
if negativeFlag == 1:
    string = "-" + string
return string

```

```
#####
### SCRIPTING ###
#####

photon_energy = 1408.1
database = "92_sm+nt_new.txt"

# First, let's find which RTAB tables are closest to the energy in question
# This should provide the best interpolation
(low_E,high_E) = findBoundingE(photon_energy,database)

# If we couldn't find data with low_E < photon_energy < high_E, then we'll just use the two nearest values
if low_E < 0 or high_E < 0:
    (low_E,high_E) = findNearestE(photon_energy,database)

print("Energies used for interpolation/extrapolation")
print("LOW: " + str(low_E) + " keV")
print("HIGH: " + str(high_E) + " keV")

# Now we want to load in the data from the two nearest-energy tables
(low_E_data,high_E_data) = getDataForInterpolation(low_E,high_E,database)

# We have the data, so it's time for the interpolation
newData = interpolate(photon_energy,low_E,low_E_data,high_E,high_E_data)

# Finally, let's output the interpolated data into its own table file
# We can reintegrate this in a new RTAB file later
output_table = open("interpolated_data.txt","w")

# Let's start with the header rows
if high_E < photon_energy: output_table.write("***BLOCK:" + str(photon_energy) + "keV   (Extrapolated from " +
str(low_E) + "keV and " + str(high_E) + "keV data)\n")
else: output_table.write("***BLOCK:" + str(float(photon_energy)) + "keV   (Interpolated from " + str(low_E) + "keV and "
+ str(high_E) + "keV data)\n")
output_table.write(" THETA   CS(B/SR)   X(1/A) A-PARALLEL-R0 (RE,IM)  A-PERPENDICULAR-R0 (RE,IM)\n")

for entry in newData:
    currentLine = ""
    for index in range(0,len(entry)):
        # We want to convert everything to scientific notation with six significant digits
        if index > 0: value = formatValue(entry[index],6)
        else:
            value = str(entry[index]) # The first entry is always an angle
            # Want to make sure the angles have 3 zero decimal points
            temp = value.split(".")
            value = temp[0] + ".000"
            # Next, we ensure the spacing is even
            while len(value) < 7:
                value = " " + value

            spacingChar = " " # Ensures that all values take the same number of spaces
            if value.startswith("-") == 0 and index > 0: spacingChar = " "
            currentLine = currentLine + spacingChar + value
    output_table.write(currentLine + "\n")
```

insert_RTAB.py

Writes interpolated RTAB data into the larger RTAB data file

This script inserts new RTAB data into a compact rtab table

```
#####
### FUNCTION DEFINITIONS ###
#####
```

```
def findE(filename):
    new_table = open(filename,"r")
    for line in new_table:
        # If the line begins with *BLOCK, we can read off the energy
        if line.startswith("*BLOCK:"):
            temp = line.split(":")
            # temp[1] is the rest of the line after *BLOCK
            temp = temp[1].split("keV")
            # Now temp[0] is the energy
            energy = temp[0]
            break
    new_table.close()
    energy = float(energy)
    return energy

def findBoundingE(photon_energy,database):
    old_table = open(database,"r")
    # Initializing high/low energy values
    high_E = -1; low_E = -1
    for line in old_table:
        # If the line begins with *BLOCK: then we have found the start of a data section
        if line.startswith("*BLOCK:"):
            temp = line.split(":")
            temp = temp[1].split("keV")
            # Get rid of the non-numerical tail
            energy = temp[0]
            energy = float(energy)
            if energy < photon_energy and energy > low_E:
                low_E = energy
            if energy > photon_energy and high_E < 0:
                high_E = energy

    old_table.close()
    return low_E,high_E

def insertData(energy,low_E,insertData,oldData,newData):
    insert_table = open(insertData,"r")
    old_table = open(oldData,"r")
    new_table = open(newData,"w")

    low_E_flag = 0 # Sets to 1 if we've read to the low_E entry in oldData
    for line in old_table:
        new_table.write(line)
        if line.startswith("*BLOCK:" + str(low_E)) == 1:
            low_E_flag = 1

    # The first blank line tells us to write the insert data
    if low_E_flag == 1 and line == " \n":
        low_E_flag = 0
        for entry in insert_table:
            new_table.write(entry)
        new_table.write("\n")
    insert_table.close()
    old_table.close()
    new_table.close()
```

```
#####
```

```
### SCRIPTING ###  
#####
```

```
# For what energy is the new data?  
energy = findE("interpolated_data.txt")
```

```
# Between which entries will we place the new data?  
(low_E,high_E) = findBoundingE(energy,"compact_92_sm+nt.txt")
```

```
# Now that we know the limits, let's insert the data  
insertData(energy,low_E,"interpolated_data.txt","compact_92_sm+nt.txt","new_92_sm+nt.txt")
```
